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MODELING MIXING-CONTROLLED REACTIVE TRANSPORT: IMPORTANCE OF COMPOUND DEPENDENT HYDRODYNAMIC AND (HYDRO)MECHANICAL TRANSVERSE DISPERSION

Gabriele Chiogna, Massimo Rolle, Olaf A. Cirpka and Peter Grathwohl

Center for Applied Geoscience, Universität Tübingen
Sigwartstrasse 10, 72076 Tübingen, Germany
e-mail: gabriele.chiogna@student.uni-tuebinge.de

Summary. Mixing processes are of utmost importance in order to understand and model reactive transport in porous media. The limiting step for reactions in groundwater systems as well as in packed bed chemical reactors is often the supply of the reaction partners and their presence at the same place. In particular, transverse mixing is a significant mechanism controlling natural attenuation of contaminant plumes at the steady state in groundwater.

In the present study, we implemented a new description of compound dependent transverse dispersion, at the porous medium continuum level, in a numerical transport code using streamline-oriented grids. Our compound-dependent parameterization of dispersion has been derived in a series of multi-tracer bench-scale experiments, recently carried out in quasi two-dimensional flow-through systems. The code was validated against the experimental results. Successively, numerical simulations were conduced in homogeneous and heterogeneous two-dimensional domains at the bench and field scale. Continuous injections of both conservative and reactive tracers were simulated. The amount of mixing was quantified by introducing a flux-related dilution index for conservative simulations, whereas the plume length was selected as comparative quantity for the reactive cases. Both methods of comparison show that the compound dependence in the mechanical dispersion term strongly influences the mixing process of the chemical species, i.e. the higher the aqueous diffusion coefficient the higher the value of the dilution index and the shorter the reactive plume.

The numerical experiments clearly indicate the importance of compound-dependent transverse dispersion for accurate modeling of mixing and reactive transport in porous media.